Technical Report

MOBILE4
Oxygenated Fuels Version
User's Guide

Ву

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MOBILE4 Oxygenated Fuels Version User's Guide

This document briefly describes changes made to the standard MOBILE4 emission factors program to create a special version which facilitates modeling the effect of the use of oxygenated fuel on carbon monoxide (CO) emissions from mobile sources. This document also explains the changes made to the MOBILE4 input and output formats to allow user input of oxygenated fuel use. Finally, examples of input and output files for the model are provided.

1.0 EFFECT ON CO EMISSIONS

The altered model calculates the effect of oxygenated fuels on CO emissions only. The adjustments used are the same as those on page 35 of the January 29, 1988 alternative fuels guidance document, "Guidance on Estimating Motor Vehicle Emissions Reductions From the Use of Alternative Fuels and Fuel Blends" (EPA-AA-TSS-PA-87-4).

Technology Specific CO Emisssion Effects of Blends
Percent Change from Gasoline

(low and high altitude)

	3.7% Oxygen*	2.0% Oxygen**
Non-catalyst Open-Loop Catalyst	-24.5% -34.9%	-13.2% -18.9%
Closed-Loop	-21.4%	-11.6%

^{* 10%} Ethanol or 5% Methanol/Cosolvent Blends

Future revisions of these numbers based on further vehicle testing are possible.

Oxygenated fuels will also affect hydrocarbon (HC) and oxides of nitrogen (NOx) emissions as well as CO emissions. However, in this version of the model, these emissions will not be assumed to be affected by the oxygen content of the fuel. Caution is necessary since no diagnostic warning of this situation is provided to the user.

^{** 11%} MTBE Blends

1.1 Fuel RVP Adjustments

MOBILE4 does not have any built-in adjustment to account for the effects of oxygenated additives on the Reid vapor pressure (RVP) of fuels. Although the model deals only with the CO emission effects of oxygenated fuels, there is some dependence of CO emissions on RVP, so the RVP effects of oxygenated fuels need to be considered. Each oxygenated additive to fuel has a different effect on RVP and the effect will depend on how the additive is blended. This report will deal with the most common additive, ethanol, in its most common blends.

There are two aspects to the RVP boost of ethanol. First, there is the RVP boost that occurs when splash-blending ethanol into gasoline to create the typical 10% blend. The January 29, 1988 document on oxygenated fuels (EPA-AA-TSS-PA-87-4) assumed that this RVP boost was 0.76 psi. This remains the current official EPA guidance. However, EPA now recognizes that this RVP boost varies with the base gasoline composition. One suggestion has been made that the RVP boost can generally be modeled simply as a function of base RVP as follows:

Delta RVP (psi) = 1.55324 - (0.07508 * base RVP)

Therefore, adding 10% ethanol to a base gasoline with 9.0 psi RVP would yield a blend of about 9.9 psi, while adding the ethanol to a base gasoline with 11.5 psi would yield a blend of about 12.2 psi. Note that the RVP inputs and outputs for the standard version of MOBILE4 are limited to a single decimal place, but this version of MOBILE4 will accept an additional decimal place and echo both decimals in the output.

RVP aspect of blend use is The second ethanol "commingling." This applies to scenarios in which ethanol blends and non-oxygenated gasoline are both available consumers at the same time of year. For instance, if ethanol blends accounted for 50% of the market, and non-oxygenated gasoline made up the other 50%, then some degree of fuel switching could occur which would result in various mixtures of gasohol and gasoline in vehicles' gas tanks. When this occurs, the resulting RVP of the mixture can be greater than a simple average of the two RVP's of the separate fuels. As a rough guideline, the maximum fleet (or fuel pool) average commingling RVP boost, which would occur at 50% market penetration of ethanol blends (and 50% non-oxygenated gasoline), assuming a 20% tank heel at refueling and some degree of brand loyalty, would be about 0.1 psi. For a 28% market penetration, the fuel pool commingling effect effect is about 0.06 psi.

It should be noted that the calculation of commingling effects gets more complex if a fuel such as an MTBE or ETBE blend is marketed simultaneously with ethanol blends and non-oxygenated gasoline. In this case the current recommended calculation procedure is given in the Guidance Document Appendix B, which is attached. Note that since this procedure is based on very limited test data, revisions may occur in the future when more test data are available.

After these two RVP adjustments (splash blending effect and commingling effect) have been calculated for the scenario of interest, they are added together and rounded to two decimal places. When these adjusted RVP values are used in the model, the added RVP can be accounted for in calculating the CO emissions. Note that no significant RVP effect is expected from the use of MTBE or ETBE blends, nor are any commingling effects of ethanol blends with MTBE blends assumed in the Guidance Document.

2.0 INPUT CHANGES

A new Table 2.2-5 (page 2-59 of the MOBILE4 User's Guide) which contains the summary of the Local Area Parameter (LAP) record is attached to this document. This page describes the LAP record with the format changes and the addition of the parameter POXY. The parameter POXY is the percent oxygen content of the fuel by weight. The oxygenate added to the gasoline can be MTBE, ETBE, ethanol, methanol or any other approved additive containing oxygen.

The input format change in the LAP record adds the percent oxygen input parameter (POXY) to the end of the record and provides for an extra digit of precision to the Base RVP (RVPBAS) and the In-use RVP (IUSRVP) parameters.

The previous FORTRAN format for the LAP record was:

(4A4, 1X, A1, F5.0, F5.0, F5.1, F5.1, 1X, I2)

It is now:

(4A4, 1X, A1, F5.0, F5.0, F5.2, F5.2, 1X, I2, 1X, F3.1)

3.0 OUTPUT CHANGES

The formats of the four output types allowed in MOBILE4 were also changed slightly. They 'echo' to the output for each scenario the percent oxygen input (POXY). For the descriptive output forms (OUTFMT = 3 or 4), POXY output can be found under the maximum temperature output. Also, the RVP inputs are now echoed to the output with two digits to the right of the decimal point instead of just one digit as in the standard MOBILE4. Examples of the descriptive output formats are attached.

The percent oxygen parameter was also 'echoed' to the output for the numerical forms (OUTFMT = 1 or 2). For both formats the parameter was placed at the end of the record. Consequently, the record lengths were increased five columns. For example, format OUTFMT = 1 increased from 221 columns to 226 columns. The outputted variable (POXY) is of FORTRAN format F3.1 and it begins on column 223 for OUTFMT = 1. The OUTFMT = 2 format increased from 140 columns to 145 columns. For OUTFMT = 2, the variable is also format F3.1 and begins in column 142.

4.0 DIAGNOSTIC MESSAGE CHANGES

For the oxygenated fuels program, a new diagnostic message was added. This message is an ERROR type and it occurs if the input percent oxygen (POXY) is less than 0.0% or greater than 3.7%. This error is fatal and no output will be obtained if these percentage bounds are not observed. The 3.7% level was selected because it is the highest oxygen percentage at which test data was collected.

The error message appears as:

M112 Error: The percent oxygen content of the fuel 3.8% is greater than 3.7% or less than 0.0%.

If the POXY parameter is omitted, the program will assign the value 0.0% to POXY and continue to run.

Table 2.2-5 (Amended)

SUMMARY OF THE LOCAL AREA PARAMETER RECORD (required in the One-time Data section if LOCFLG = 2, and required in the Scenario Data section if LOCFLG = 1)

<u>Field</u>	Content, Variable Name, Codes	<u>Format</u>	Available Values	Refer to Section
1	Scenario Name (SCNAME)	4A4,1X	N/A	2.2.9
2	ASTM volatility class (ASRMCL)	Al	A,B,C,D,E	2.2.10
3	Minimum daily temperature (TEMMAX), in °F	F5.0	0100.	2.2.11
4	Maximum daily temperature	F5.0	0120.	2.2.11
	(TEMMIN and TEMMAX are used in diurnal index calculations for		tive HC emiss	sions.
5	Base RVP (RVPBAS), in psi (currently average fuel volatility for the geographic area of interest)	F5.2	7.0-15.2	2.2.12
6	In-use RVP (IUSRVP) in psi (Volatility fuel volatility limit after implementation of in-use volatility control in the geographic area of inte	F5.2,1X	7.0-15.2	2.2.13
7	In-use start year (IUSESY) (Last 2 digits of first calend year of in-use fuel volatility		89-99,	2.2.13
8	Percent Oxygen (POXY) by weight of the fuel blend	1X,F3.1	0.0-3.7 At	tachment